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Title: ACADEMIC RESEARCH TOPICS FOR THE ADVANCED ACCELERATOR APPLICATIONS PROJECT

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This document is a compilation of research topics that are appropriate for execution at universities and by graduate students. It was developed from contributions from technical specialists at Los Alamos National Laboratory and Argonne National Laboratory.

Academic Research Topics for the Advanced Accelerator Applications Project

(Denis Beller, AAA University Programs Lead, Dec. 2001)

Introduction

The Office of Nuclear Energy, Science, and Technology of the Department of Energy is managing an Advanced Accelerator Applications (AAA) Program to develop a new technology for treatment of used nuclear fuel. The main focus of this effort is on Accelerator-driven Transmutation of Waste (ATW) (transmutation is a nuclear process to produce short-lived or non-radioactive materials from high-level radioactive waste). The AAA Project and ATW studies involve three major technologies to care for a major portion of used nuclear fuel: separations and waste forms, accelerators, and transmuters (proton-neutron target and sub-critical blanket). Significant research and development must be conducted to realize the goals of the AAA Project, and universities, faculty, and students are playing a major role in conducting that research.

The research topics listed below are intended for conduct by undergraduate and graduate-level students as well as in post-doctoral appointments. This research could be conducted in a student-based research project at a university, or it could involve introductory assignments at a national laboratory, following which the student could return to the university setting for completion on a semi-independent basis. Summer assignments would be ideal for the introductory phase and could include faculty appointments to facilitate student guidance at the university. Laboratory research locations are Los Alamos National Laboratory (LANL, north of Santa Fe, NM), Argonne National Laboratory (ANL, near Chicago, IL or in Idaho), Lawrence Livermore National Laboratory (LLNL, east of Oakland, CA), and Savanah River Site (SRS, near Aiken, SC and Savanah, GA).

Table I.
List of Research Project Topics (click to go to description)

Research Project Topics

Systems Engineering and Analysis

Description: Systems studies are being used to assess readiness level of various technologies and to integrate different components and processes (e.g., separations with transmuters and fuels). Students can contribute by helping AAA researchers establish performance objectives, assess phenomena sensitivities, assess component sensitivities, optimize component performance, integrate components into subsystems and assess subsystem sensitivities, optimize subsystem performance, integrate subsystems into systems and assess system sensitivities, and optimize overall system performance.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: A variety of engineering disciplines: nuclear, systems, mechanical, electrical, etc.
Potential summer research locations: LANL, ANL
Security and access requirements: U.S. citizen, no clearance

Separations of Used Nuclear Fuel from LWR, Transmutation, and Other Fuel Cycles

Description: This topic, AAA Separations Technology, is for research and development of methods and processes to separate transuranic elements and long-lived fission products from nuclear fuel that has been discharged from commercial light water reactors in the U.S., as well as that discharged from reactors for the transmutation of nuclear waste. Two candidate technologies are currently being investigated: UREX (like PUREX but without separation of plutonium from other higher actinides), and pyro-processing using molten salt and electric fields. Considerable work must be done to transition these concepts to production facilities. Requirements include compiling data, developing process models, performing systems engineering studies, and conducting laboratory experiments.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear, or chemical, or radio-chemical engineering, chemistry, radiochemistry.
Potential summer research locations: ANL, SRS
Security and access requirements: U.S. citizen, no clearance

Further descriptions of specific separations research topics.

- Light Water Reactor Fuel Treatment: Modeling of UREX solvent extraction process. Preparation of chemical properties data table for the Generic UREX Model (GUM); literature search for solubilities, reaction rates, extractant/complexant behavior, etc. UREX process optimization using the GUM; reagent selection, acid concentrations, flow rates, etc.
- Advanced Spent Fuel Treatment Process: Tabulation of chemical thermodynamics data for actinide and fission product fluorides from search of open literature. Application of data to design and analysis of fluoride volatility process for spent fuel treatment.
- Process Systems Engineering: Perform systems engineering study of AAA separations and fuel fabrication processes to identify areas for focus of technology development activities. Apply systems engineering model to identify optimum scale and siting of various separations and fabrication processes.
- Partitioning and Transmutation Criteria: Establish objective criteria for actinide and long-lived fission product recovery and transmutation using Yucca Mountain Project models as a basis or starting point.
- Iodine Recovery for Transmutation: Model process steps for (1) removing iodine (I_2) from UREX dissolver solution by sparging with oxides of nitrogen, (2) desorbing iodine from collector, and (3) conversion of I_2 to NaI. Test model with bench-scale experiments.
- Development of Iodine Transmutation Target: Develop model for NaI transmutation target behavior through long-term tests of irradiation capsules in a laboratory environment at representative target compositions and operating temperatures. Evaluate chemical and physical interactions of the target material with the container material and develop recommendations for material selection (container material).
- Waste Form Processing and Characterization: Develop process for synthesis of flourapatite with additions of salts of alkali metal, alkaline earth, and lanthanide fission products. Characterize the microstructure of the synthesized waste form and perform controlled leaching experiments for prediction of waste form durability in a representative repository environment.

Fabrication of Nuclear Fuel for ATW Systems

Description: Fuel development activity for accelerator driven transmutation systems involves development of fuel fabrication processes for actinide-bearing fuel, investigation of out-of-pile thermal behavior, measurement of

thermo-physical properties of fuel, studies of in-reactor fuel behavior, fuel performance modeling, and fuel fabrication process scale-up. Several different fuel concepts are being considered for transmutation, including oxide-, nitride-, and metal-based fuels in monolithic and dispersed forms. Potentials coolants are lead-bismuth, sodium, and gas. Data on fuel physical properties, irradiation behavior, and behavior during fabrication need to be acquired. Students can contribute by conducting technical reviews of the various fuel options, by performing laboratory scale experiments and data analysis, by formulating a fuel performance code framework and developing mechanistic models for observed fuel phenomena, and by participating in irradiation testing and post-irradiation examination. Comprehensive investigation of these topics is on the level of M.S.- and Ph.D.-level research. Some of the broad research areas listed here will be narrowed based on the interest and experience of the student and on program priorities.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear, or chemical, or radio-chemical engineering, chemistry, radiochemistry.
Potential summer research locations: ANL, SRS
Security and access requirements: U.S. citizen, no clearance

Fabrication Process Scaleup Studies: Design of production-scale remote fuel fabrication processes for ATW initial feed and recycle material. Estimation of capital and operating costs for fabrication of oxide, nitride, and metallic fuel in monolithic form and for metal matrix and coated particle dispersion fuel. Identification of areas on which to focus fabrication technology development.
Academic Level: graduate
Academic Discipline: Materials Science, Nuclear Engineering, Physics, Solid State Chemistry.
Potential summer research locations: ANL-W
Security and access requirements: U.S. Citizen, no clearance

Metal Fuel Casting Process Development: Design of laboratory scale process for metallic fuel pins that incorporate volatile actinides. Conceptual system design. Laboratory scale testing of concepts and components. Assembly and testing of laboratory scale casting system using non-radioactive surrogate materials. Identification of areas on which to focus technology development for process scale-up.
Academic Level: graduate
Academic Disciplines: Material Science, Nuclear Engineering, Physics, Solid State Chemistry
Potential summer research locations: lab
Security and access requirements: U.S. citizen, no clearance

Metal Matrix Dispersion Fuel Process Development: Fabrication and characterization of surrogate metal matrix dispersion fuel specimens using non-radioactive materials. Fabrication process development. Conceptual design of a product scale system including estimation of capital and production cost. Identification of issues in fabrication of minor actinide-bearing fuel.
Academic Level: graduate
Academic Disciplines: Material Science, Nuclear Engineering, Physics, Solid State Chemistry
Potential summer research locations: ANL-W
Security and access requirements: U.S. citizen, no clearance

High Temperature Gas Reactor Fuel Process Development: Fabrication and characterization of surrogate gas reactor fuel specimens using non-radioactive materials. Development of alternate particle coating technology, alternative coating materials, and alternative fuel particles compositions. Identification of issues in fabrication of minor actinide-bearing gas reactor fuel. Identification of issues affecting fuel performance.
Academic Level: graduate
Academic Disciplines: Material Science, Nuclear Engineering, Physics, Solid State Chemistry
Potential summer research locations: ANL-W
Security and access requirements: U.S. citizen, no clearance

Coating Processes for Fuel Particles: Develop coating processes for fuel particles to be incorporated into matrix dispersion fuel. Identification of coating materials, development of coating deposition process through analysis and laboratory scale experiments. Quantification of the parameters affecting coating process. Identification of areas for further technology development.
Academic Level: undergraduate, graduate, post-doc

Academic Discipline: Materials Science, Nuclear Engineering, Physics, Solid State Chemistry
Potential summer research locations: ANL-W, ANL-E
Security and access requirements: U.S. citizen, no clearance

Metal Fuel Phase Equilibria: Establish phase equilibria data for metal alloys in the composition ranges of interest for ATW initial LWR feed and equilibrium recycle fuels. Measure liquidus and solidus temperatures, determine phase arrays, and investigate effects of alloying elements. Measurement of thermodynamic properties.
Academic Level: graduate, post-doc, Ph.D
Academic Discipline: Materials Science, Nuclear Engineering, Physics, Solid State Chemistry
Potential summer research locations: lab
Security and access requirements: U.S. citizen, Q clearance preferred but not required.

Further descriptions of specific fuel-fabrication research topics.

- Fabrication Process Scale-up Studies: Design of production-scale remote fuel fabrication processes for ATW initial feed and recycle material. Estimation of capital and operating costs for fabrication of oxide, nitride, and metallic fuel in monolithic form and for dispersion fuel. Identification of areas on which to focus fabrication technology development.
- Metal Fuel Casting Process Development: Design of a laboratory scale process for melt casting of metallic fuel pins that incorporate volatile actinides. Conceptual system design. Laboratory scale testing of concepts and components. Assembly and testing of laboratory scale casting system using non-radioactive surrogate materials. Identification of areas on which to focus technology development for process scale-up.
- Fuel Performance Modeling: Development or modification of existing empirical correlations and mechanistic models (as appropriate) to describe major fuel phenomenology such as material property changes, component redistribution, fission gas behavior, and fuel swelling for candidate fuel types. Inclusion of these models into a code framework incorporating thermal calculations. Code validation by comparison of model predictions with postirradiation data.
- Coating Processes for Fuel Particles: Develop coating processes for fuel particles to be incorporated into metal matrix dispersion fuel. Identification of coating materials, development of coating deposition process through analysis and laboratory scale experiments. Quantification of the parameters affecting coating process. Identification of areas for further technology development.
- Metal Fuel Phase Equilibria: Establish phase equilibria data for metal alloys in the composition ranges of interest for ATW initial LWR feed and equilibrium recycle fuels. Measure liquidus and solidus temperatures, determine phase arrays, and investigate effects of alloying elements.
- Fuel Irradiation Testing: Assist in design, analysis, and postirradiation examination of fuel irradiation tests. Safety analysis, thermohydraulic calculations, and interpretation of postirradiation data. Provide data and assist in validation of fuel performance code.
- Fuel Cladding Chemical Interaction Studies: Use out-of-pile testing to determine the compatibility of proposed fuel types with proposed cladding materials. Use of diffusion couples to quantify penetration rates, phases formed, and evaluation of effect of interaction on fuel performance.

Coolant Technology for ATW Target/Window and Blanket Systems

Description: Coolants currently being considered include sodium, helium, lead-bismuth eutectic (LBE), and others. The student can contribute in the following areas: identify candidate coolants, evaluate possible coolant options (address availability), perform sensitivity and trade-off studies with reference to preliminary design criteria, quantify relevant properties via laboratory experiments (out-of-pile or separate effect), quantify coolant performance in a proton/neutron flux environment* (not necessarily prototypic), quantify coolant performance in contact with the prototypic materials in a proton/neutron environment* (not necessarily prototypic), perform scaled experiments in a prototypic proton/neutron environment* in preparation for larger scale demonstration.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear, chemical or mechanical engineering, chemistry, radiochemistry.
Potential summer research locations: LANL, ANL
Security and access requirements: U.S. citizen, no clearance

Further descriptions of specific Target/Blanket coolant technology research topics.

- **Lead-Bismuth experiments (LBE) at UNLV**: Perform complementary experiments to LBE at LANL. Commission the LBE loop from Russia. Test oxygen probes in LBE loop. Test corrosion probes in LBE loop.

Perform corrosion and supporting technologies. Perform T–H tests (local HTC). Write analysis report. Publish results.

- **Study methodology of producing corrosion probes**: Determine ideal manufacturing process for producing high quality corrosion probes. Study current methodology of producing corrosion probes. Devise new technique for producing corrosion probes which addresses current manufacturing shortcomings. Manufacture corrosion probes utilizing old technique. Manufacture corrosion probes utilizing new technique. Test corrosion probes in an irradiation environment. Perform metallography on probes. Write analysis report. Publish results.
- **Study methodology of producing oxygen probes**: Determine ideal manufacturing process for producing high quality oxygen probes. Study current methodology of producing oxygen probes. Devise new technique for producing oxygen probes which addresses current manufacturing shortcomings. Manufacture oxygen probes utilizing old technique. Manufacture oxygen probes utilizing new technique. Test oxygen probes in irradiative environment. Perform metallography on probes. Write analysis report. Publish results.

Fuel Performance Studies

Description: Development or modification of existing empirical correlations and mechanistic models (as appropriate) to describe major fuel phenomenology such as material property changes, component redistribution, fission gas behavior, and fuel swelling for candidate fuel types. Inclusion of these models into a code framework incorporating thermal calculations. Code validation by comparison of model predictions with postirradiation data.
Academic Level: graduate, post-doc, Ph.D.
Academic Disciplines: Materials Science, Nuclear Engineering, Physics, Solid State Chemistry
Potential summer research locations: ANL-W, labs
Security and access requirements: U.S. citizen, no clearance

Further descriptions of specific fuel performance research topics.

- **Fuel Irradiation Testing:** Assist in design, analysis, and post-irradiation examination of fuel irradiation tests. Safety analysis, thermohydraulic calculations, and interpretation of post-irradiation data. Provide data and assist in validation of fuel performance code.
- **Fuel Cladding Chemical Interaction Studies:** Use out-of-pile testing to determine the compatibility of proposed fuel types with proposed cladding materials. Use of diffusion couples to quantify penetration rates, phases formed, and evaluation of effect of interaction on fuel performance.
- **Advanced Cladding Development:** Survey and evaluation of the suitability advanced steel cladding for transmuter fuels. Mechanical and physical properties testing of materials. Irradiation damage and lifetime calculations. Possibility for irradiation testing and post-irradiation examination.

Materials Technology for ATW Target/Window and Blanket Systems

Description: Many different materials are being investigated in support of the AAA project. Students can contribute in the following areas: identify candidate materials, evaluate possible material options (address availability and fabricability) , perform sensitivity and trade-off studies with reference to preliminary design criteria, quantify relevant properties quantified via laboratory experiments (out-of-pile or separate effect) , quantify material performance in a proton/ neutron flux environment (not necessarily prototypic), quantify material performance in contact with the prototypic coolant in a proton/neutron environment (not necessarily prototypic), perform scaled experiments in a prototypic proton/neutron environment in preparation for larger scale demonstration.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear or mechanical engineering, materials science and engineering, physics.
Potential summer research locations: LANL, ANL
Security and access requirements: U.S. citizen, no clearance

Neutronic and Mechanical Coupling of ATW Target and Blanket

Description: A critical challenge is to couple the proton/neutron target to the surrounding blanket, both neutronically and physically. We must produce as many neutrons as possible in the target, then ensure they reach the fuel in the subcritical blanket, while simultaneously ensuring that all materials are compatible. Students can identify and evaluate concepts for coupling targets and blankets, perform sensitivity and trade-off studies with reference to preliminary design criteria, test the coupling concepts in laboratory scale tests (small accelerators or LANSCE), and perform scaled coupling tests addressing dominant phenomenology. Students could also evaluate concepts for future large-scale experiments addressing multiple phenomena or scaled experiments in a high-powered accelerator facility in preparation for a larger-scale demonstration.

Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear, chemical or mechanical engineering.
Potential summer research locations: LANL, ANL
Security and access requirements: U.S. citizen, no clearance

Heat Removal Technology for ATW Target/Window and Blanket Systems

Description: Another critical element of an accelerator-driven transmutation system will be the heat removal system. Students might identify or evaluate loop concepts for different coolants, perform sensitivity and trade-off studies with reference to preliminary design criteria, test loop concepts in laboratory scale tests (cold tests), conduct scaled heat removal tests (by using electrical heating) to address dominant phenomenology, conduct large scale experiments to address multiple phenomena (including transients), or develop concepts for scaled experiments in a nuclear facility (including bulk heating) in preparation for larger-scale demonstration tests.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear or mechanical engineering.
Potential summer research locations: LANL, ANL
Security and access requirements: U.S. citizen, no clearance

Waste Forms for Disposal of Separated Isotopes and Processing Wastes

Description: One of the major contributions that the AAA Project may make to the nation's ability to permanently dispose of nuclear waste will be in the form of more robust waste forms. Students may contribute in basic concept development, flow-sheet development, scoping experiments with simulated fission product content, Waste Acceptance Criteria (WAC) evaluation, confirmation of process chemistry, bench-scale or engineering-scale testing, testing with simulated waste streams, preliminary testing of equipment design concepts, process validation, short-term waste form characterization, initial model development, process validation through unit operations. testing at engineering scale with representative radioactive fission product and actinide content, and use of existing hot cell facilities.
Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: nuclear, chemical or mechanical engineering, chemistry, radiochemistry.
Potential summer research locations: LANL, ANL
Security and access requirements: U.S. citizen, no clearance

Accelerator Technology for Transmutation Systems

Description: The ATW and the ADTF will require advances in accelerator technology (control, beam energy, beam power, diagnostics, beam transport modeling, etc.). This could include modeling radio-frequency quadropoles (RFQ), experiments with the Low Energy Demonstration Accelerator (LEDA) and/or the Low Energy Beam Transport (LEBT), design and optimization of components,

Further descriptions of specific fuel-fabrication research topics.

- Simulation and Optimization of LEBT Beam Transport: Qualify and improve theoretical model of space-charge dominated transport in the LEDA / LEBT. Use PARMELA and/or PBGUNS codes to investigate and optimize beam transport in the LEBT. Compare to experimental data where possible and identify the salient experimental parameters involved in linearizing the beam phase-space delivered to the LEDA RFQ. Provide an input for the RFQ model. Identify relevant experiments that can be carried out to verify the code.
- Simulation of RFQ Performance: Compare simulation results with experimental data for the LEDA RFQ. Use TOUTATIS and/or PARTECHM codes to investigate and optimize beam transport through the LEDA RFQ. Compare to experimental data and study the effects of RFQ field level and matching. Provide detailed phase space pictures for comparison to existing experimental data. Identify relevant experiments that can be carried out to verify the code.
- Determine optimal fit to halo measurement data using full transport model: Use the LINAC code or equivalent to determine the best model of the beam phase-space consistent with existing experimental data. Use tomographic and/or maximum entropy methods to generate a semi-empirical phase space fit.

Academic Level: undergraduate, graduate, post-doc.
Academic Disciplines: electrical, electronic, or mechanical engineering, physics.
Potential summer research locations: LANL
Security and access requirements: U.S. citizen, no clearance